

the Vainshtein-Presnyakov-Sobelman (VSP) approximation [4] and Glauber approximation [7]. Saxena *et al* [8] performed the calculation of excitation of the hydrogen atom from its ground as well as from metastable state by positron impact in the framework of distorted wave approximation in which distorted wave in initial and final channel is the Coulomb wave involving screening parameters following Junker [9]. Recently, Verma and Srivastava [10] have carried out calculations for positron impact excitation of hydrogen from the metastable  $H(2s)$  state in distorted wave approximation. They have taken distortion potential (static potential of the final channel) to be the same in both the initial and final channels.

There are some elaborate calculations for the excitation of metastable hydrogen atom by electron impact (see [11–17]) out of which the works of Odgers *et al* are expected to be most accurate, who have employed a modified version of IERM approach. The elaborate calculation is difficult to extend to atoms containing more than one electron. It is always suggested to find simple model to provide reliable results at intermediate and high energies. Moreover, the works reported so far indicate that not much attention has been paid to the study of positron impact excitation of hydrogen from the metastable  $H(2s)$  state.

In our earlier work, we have investigated the inelastic scattering of electron by the  $H(2s)$  metastable state [18–20]. We have employed a distorted wave method based on two potential formalism. The  $H(2s) \rightarrow H(3s)$  integrated excitation cross sections are in excellent agreement with those of most elaborate calculations of Odgers *et al* and Callaway *et al* at incident energies 20 eV and above [18]. We reported earlier the differential cross sections for  $H(2s) \rightarrow H(3s)$  excitation due to electron and positron impact and interesting features have been observed [19]. Later on the calculations have been extended to electron impact differential cross sections for higher excitations [20]. The success of our work in case of electron impact has encouraged us to undertake the theoretical investigations of positron impact excitation of hydrogen atom from the metastable  $H(2s)$  state.

In the present study, we have used distorted wave model arising out of the two potential approach. We consider distortion in both the channels. The continuum wave functions are obtained in the presence of an arbitrary potential which is spherically symmetric and satisfies the asymptotic condition. Our arbitrary potential for both the channels is chosen as the static potential of the initial metastable state. This is procedure adopted in the First Order Many Body Theory (FOMBT) approach. Several theoretical investigations have revealed that the use of final state distorting potential for both channels provides better agreement with the experimental data for excitation of  $p$ -states. Since the present finding is mainly concerned with excitation of  $s$ -state, we have used the initial state distorting potential for both the channels. The contribution of polarization in the present calculation is expected to be small. Keeping in view the use of simplified model, the polarization potential has not been included in distortion potential in the present work.

## 2. Theory

We briefly discuss the theory of the distorted wave method used in the present work. The total Hamiltonian for the positron-hydrogen system is expressed as

$$H = H_0 + H_{at} + V, \quad (1)$$

where  $H_0$  is the Hamiltonian of the free incident particle and  $H_{at}$  that of the target atom. The interaction potential is expressed as

$$V = \frac{z}{x} - \frac{1}{|x-r|}. \quad (2)$$

In the framework of 'two-potential approach', the exact  $T$ -matrix from the initial state  $|\phi_i\rangle$  with momentum  $k_i$  to the final state  $\langle\phi_f|$  with momentum  $k_f$  is given by

$$T_{if} = \langle\chi_f^- \phi_f|V-U_f|\psi_i^+\rangle + \langle\chi_f^- \phi_f|U_f|\beta_i \phi_i\rangle, \quad (3)$$

where  $\beta_i$  is the initial state plane wave,  $\psi_i^+$  is the initial state full scattering wave function which satisfies the Schrödinger equation

$$(H-E)\psi_i^+ = 0 \quad (4)$$

The (+) superscript symbolizes the usual outgoing wave boundary condition.  $U_f$  is chosen as a spherically symmetric arbitrary distorting potential and satisfies the required boundary conditions. The potential  $U_f$  is also used to calculate  $\chi_f^-$  i.e.,

$$(H_0 + U_f - E_f)\chi_f^- = 0, \quad (5)$$

where superscript (-) corresponds to the incoming wave boundary condition. One cannot evaluate eq. (3) without making some approximation as  $\psi_i^+$  cannot be evaluated exactly in practice. The full scattering wave function for the initial state can be expanded in terms of the full Green's function  $G^+$  as

$$|\psi_i^+\rangle = |\phi_i \chi_i^+\rangle + G^+(V-U_i)|\phi_i \chi_i^+\rangle, \quad (6)$$

where  $\chi_i^+$  is solution of the Schrödinger equation

$$(H_0 + U_i - E_i)\chi_i^+ = 0. \quad (7)$$

Here,  $U_i$  is also an arbitrarily chosen spherically symmetric distorting potential which satisfies the asymptotic condition. We consider the process of excitation only. Using eq. (6) and the expansion of Green's function the first order distorted wave transition matrix element takes the form

$$T_{if} = \left\langle \chi_f^- \phi_f \left| \frac{1}{|x-r|} \right| \phi_i \chi_i^+ \right\rangle. \quad (8)$$

In the present study, we have taken the 2s state of the hydrogen atom as the initial metastable state. We evaluate the scattering amplitude by using partial wave analysis.

The initial and final channel continuum wave functions are calculated numerically using variable step size numerov method. The radial integration has been carried out upto 120 atomic units having the initial step size 0.01. At the highest energy for  $s$ - $s$  transition, calculations upto angular momentum  $l = 30$  has been carried out whereas for  $s \rightarrow p$  transition the corresponding angular momentum is 50. Higher partial wave contributions are substituted by the Born term whenever required.

### 3. Results and discussion

We calculate TCS for the scattering of positron by metastable  $2s$ -state of the hydrogen atom in the energy region 20–200 eV. Results of FBA has also been calculated. The present model is expected to be valid for intermediate energy regions. The minimum energy at which this method predicts reliable results is not certain. In our earlier investigation on electron-hydrogen scattering  $2s \rightarrow 3s$  excitation results of the present method are found to be in excellent agreement with those of most elaborate calculation by Odgers *et al* for incident energies 20 eV and above. Our choice of energy depends on our earlier finding. Results of FBA have been calculated with and without partial wave to check the programme for distorted wave calculations.

In Figure 1, we have compared our integrated cross sections for  $2s \rightarrow 3s$  excitation with those of electron impact. It has been found that the present positron results are slightly higher than the earlier findings in case of electron scattering. The initial and the final channel distorted waves are calculated using the repulsive static potential in the case of positron, whereas in the case of electron corresponding attractive potential is employed. Difference between two sets of results is probably due to this reason.

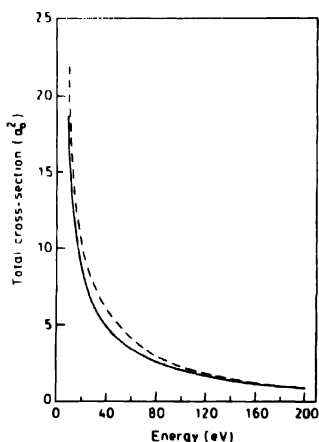


Figure 1. Total cross sections for the  $2s \rightarrow 3s$  excitation of hydrogen atom by electron and positron impact in units of  $a_0^2$ : —, electron result, - - - - present positron result.

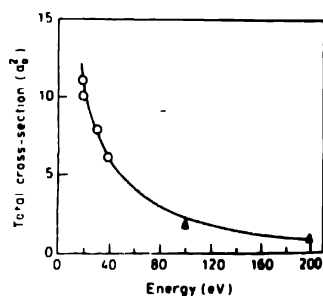


Figure 2. Total cross sections for the  $2s \rightarrow 3s$  excitation of hydrogen atom by positron impact in units of  $a_0^2$ : — present positron result,  $\circ$ ,  $\Delta$  Verma and Srivastava [10];  $\blacktriangle$  Saxena *et al* [8].

In Figure 2, we compare our results for  $2s \rightarrow 3s$  excitation with those of Saxena *et al* [8] and Verma and Srivastava [10] in the energy region 20–200 eV. Saxena *et al* [8] have carried out calculation in the energy region 100–500 eV, whereas Verma and Srivastava [10] have reported results for incident energies below 40 eV. In the incident energy region 100–200 eV the present results coalesce with those of Saxena *et al*. In the energy region 20–30 eV the results of Verma and Srivastava differ by 10% from those of ours. This might be due to the fact that Verma and Srivastava have employed final state static potential in calculating the distorted wave. Overall comparison suggests that present distorted wave method although very simple predicts reliable results in the energy region considered.

We have also calculated the cross section for  $2s \rightarrow ns$  ( $n = 4, 5, 6$ ) transition in the same energy region. Saxena *et al* have also calculated  $2s \rightarrow 4s$  excitation cross sections in the incident energy region 100–500 eV. At 100 and 200 eV present  $2s \rightarrow 4s$  results are in good agreement (not shown here) with those of Saxena *et al* (Model BC 1) [8]. In Tables 1–4, we have presented the TCS for  $2s \rightarrow ns$  ( $n = 3, 4, 5, 6$ ) transitions in the energy

**Table 1.** Total cross sections for the  $2s \rightarrow 3s$  excitation of the hydrogen atom in units of  $a_0$ .

$E$ (eV)	FBA	DW (positron)	DW (electron)
10.0	0.198 E + 02	0.407 E + 02	0.192 E + 02
20.0	0.106 E + 02	0.112 E + 02	0.102 E + 02
30.0	0.726 E + 01	0.753 E + 01	0.705 E + 01
40.0	0.550 E + 01	0.565 E + 01	0.538 E + 01
50.0	0.443 E + 01	0.452 E + 01	0.435 E + 01
80.0	0.280 E + 01	0.282 E + 01	0.276 E + 01
100.0	0.225 E + 01	0.226 E + 01	0.222 E + 01
150.0	0.150 E + 01	0.151 E + 01	0.149 E + 01
200.0	0.113 E + 01	0.113 E + 01	0.112 E + 01

**Table 2.** Total cross sections for the  $2s \rightarrow 4s$  excitation of the hydrogen atom in units of  $a_0^2$ .

$E$ (eV)	FBA	DW (positron)	DW (electron)
10.0	0.382 E + 01	0.440 E + 01	0.398 E + 01
20.0	0.207 E + 01	0.223 E + 01	0.197 E + 01
30.0	0.141 E + 01	0.148 E + 01	0.137 E + 01
40.0	0.107 E + 01	0.111 E + 01	0.105 E + 01
50.0	0.863 E + 00	0.888 E + 00	0.850 E + 00
80.0	0.545 E + 00	0.553 E + 00	0.538 E + 00
100.0	0.437 E + 00	0.442 E + 00	0.432 E + 00
150.0	0.293 E + 00	0.294 E + 00	0.290 E + 00
200.0	0.220 E + 00	0.220 E + 00	0.218 E + 00

region 10–200 eV for electron and positron impact alongwith FBA results. It is found that electron and positron results exhibit similar trend as observed in Figure 1. To the best of our knowledge, there is no other theoretical work for positron impact in case of  $2s \rightarrow 5s$  and  $2s \rightarrow 6s$  excitations.

**Table 3.** Total cross sections for the  $2s \rightarrow 5s$  excitation of the hydrogen atom in units of  $a_0^2$ .

$E$ (eV)	FBA	DW (positron)	DW (electron)
10.0	0 145 E + 01	0.168 E + 01	0 162 E + 01
20.0	0 787 E + 00	0 851 E + 00	0.750 E + 00
30.0	0.538 E + 00	0.556 E + 00	0.552 E + 00
40.0	0 408 E + 00	0.424 E + 00	0.400 E + 00
50.0	0.328 E + 00	0 338 E + 00	0.323 E + 00
80.0	0 207 E + 00	0 211 E + 00	0.205 E + 00
100.0	0.166 E + 00	0.168 E + 00	0 164 E + 00
150.0	0.111 E + 00	0.112 E + 00	0.110 E + 00
200.0	0 837 E - 01	0.838 E - 01	0.828 E - 01

**Table 4.** Total cross sections for the  $2s \rightarrow 6s$  excitation of the hydrogen atom in units of  $a_0^2$ .

$E$ (eV)	FBA	DW (positron)	DW (electron)
10.0	0.710 E + 00	0 843 E + 00	0.840 E + 00
20.0	0 392 E + 00	0.425 E + 00	0.321 E + 00
30.0	0.268 E + 00	0.282 E + 00	0.249 E + 00
40.0	0.203 E + 00	0.211 E + 00	0.189 E + 00
50.0	0.164 E + 00	0 169 E + 00	0 152 E + 00
80.0	0.103 E + 00	0 105 E + 00	0.101 E + 00
100.0	0.829 E - 01	0.839 E - 01	0 834 E - 01
150.0	0.556 E - 01	0.558 E - 01	0 553 E - 01
200.0	0.417 E - 01	0.418 E - 01	0.412 E - 01

Our results for  $2s \rightarrow 3p$  excitation cross section by positron impact in the energy range 20–200 eV have been plotted in Figure 3 along with those of Verma and Srivastava which are available upto incident energy 40 eV only. At the incident energy 40 eV, the result coalesces with that of Verma and Srivastava [10] and below this energy, their results are slightly higher than the present predictions.

We report the differential cross sections for ( $2s \rightarrow 3s$ ), ( $2s \rightarrow 4s$ ) and ( $2s \rightarrow 5s$ ) transitions in  $e^+H$  scattering. In Figures 4 and 5 we have plotted the differential cross sections for the  $2s \rightarrow ns$  ( $n = 3, 4, 5$ ) transitions for two different energies. The features for all the above mentioned transitions have been found to be the same. In  $s \rightarrow s$  transition at low energy, say 20 eV two zeros in the angular distribution has been noticed for excitations

to 3 s, 4 s and 5 s states. With the enhancement of energy say 50 eV, we find three zeros. In our earlier communication, this feature has already been noticed. At low energies the distorted wave results for electrons including exchange do not predict any minimum though

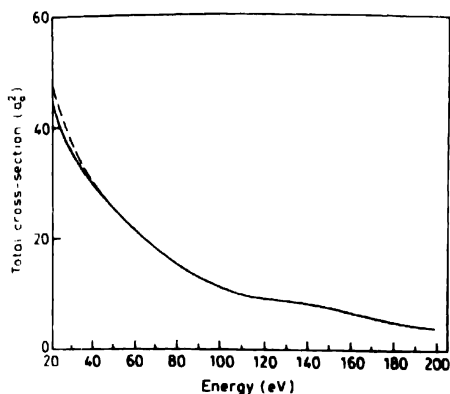


Figure 3. Total cross sections for the  $2s \rightarrow 3p$  excitation of hydrogen atom by positron impact in units of  $a_0^2$  present positron result; - - - - Verma and Srivastava [10]

at some higher energy they predict a minimum. It has been found that electron results show similar enhancement of minima with increase in energy as enhancement of zero in case of

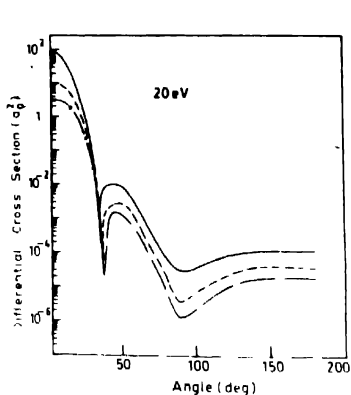


Figure 4. Differential cross sections for the  $2s \rightarrow ns$  ( $n = 3, 4, 5$ ) excitation of hydrogen atom by positron impact in units of  $a_0^2$ . —,  $2s \rightarrow 3s$ ; - - -  $2s \rightarrow 4s$  and — · —  $2s \rightarrow 5s$  at incident energy 20 eV.

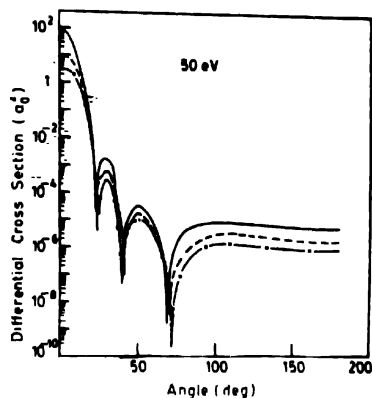


Figure 5. Same as in Figure 4 at incident energy 50 eV.

positrons. In the case of FBA two zeros in the DCS have been observed. The presence of minima or zeros has been attributed to the nodal properties of the target wave functions (see [19]). From a close inspection of the results obtained, it is concluded that more elaborate theoretical calculations and experimental investigations are required to understand the dynamics of the system properly.

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